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Structure of S-matrices for three body Schrödinger operators

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1. Results

We consider a collision process of quantum mechanical three particles moving in \mathbf{R}^3 . Suppose in the initial state two of them form a bound state and in the final state all of the three particles move freely. The aim of this paper is to study some properties of the scattering operator associated with this process. Consider three particles with mass m_i , position x^i . We choose a pair (i, j) arbitrarily and denote it by α . Let

$$\frac{1}{m_\alpha} = \frac{1}{m_i} + \frac{1}{m_j}, \quad \frac{1}{n_\alpha} = \frac{1}{m_k} + \frac{1}{m_i + m_j},$$

$$x^\alpha = \sqrt{2m_\alpha}(x^i - x^j), \quad x_\alpha = \sqrt{2n_\alpha}\left(x^k - \frac{m_i x^i + m_j x^j}{m_i + m_j}\right).$$

Let $X = \{(x^1, x^2, x^3); \sum_{i=1}^3 m_i x^i = 0\}$. Then in $L^2(X)$ our Schrödinger operator is given by

$$H = H_0 + \sum_{\alpha} V_{\alpha}(x^{\alpha}), \quad H_0 = -\Delta_{x^{\alpha}} - \Delta_{x_{\alpha}}.$$

We impose the following assumption on the potential V_{α} :

$$V(x) \text{ is a real-valued smooth function on } \mathbf{R}^3, \\ \text{and } |\partial_y^m V_{\alpha}(y)| \leq C_m (1 + |y|)^{-\rho - m}, \rho > 0, m = 0, 1, 2, \dots$$

We introduce wave operators. Let $\rho > 1$ and

$$W_0^{\pm} = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0}, \quad W_{\alpha}^{\pm} = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH} e^{-itH_{\alpha}} J_{\alpha},$$

where

$$H_{\alpha} = H_0 + V_{\alpha}, \quad (J_{\alpha} f)(x^{\alpha}, x_{\alpha}) = \varphi^{\alpha}(x^{\alpha}) f(x_{\alpha}),$$

φ^{α} being an eigenfunction of $h^{\alpha} = -\Delta_{x^{\alpha}} + V_{\alpha}(x^{\alpha})$ with eigenvalue $E^{\alpha} < 0$. Let

$$S_{0\alpha} = (W_0^+)^* W_{\alpha}^-$$

be the scattering operator. To introduce the S-matrix, it is necessary to consider the Fourier transform. For $f \in L^2(\mathbf{R}^6)$, we set

$$(F_0 f)(\lambda, \theta) = (2\pi)^{-3} 2^{-1/2} \lambda \int_{\mathbf{R}^6} e^{-i\sqrt{\lambda}\theta \cdot x} f(x) dx.$$

Then F_0 is a unitary operator from $L^2(\mathbf{R}^6)$ to $L^2((0, \infty); L^2(S^5))$. We also define for $f \in L^2(\mathbf{R}^3)$,

$$(F_{0\alpha} f)(\lambda, \omega) = (2\pi)^{-3/2} 2^{-1/2} (\lambda - E^\alpha)^{1/4} \int_{\mathbf{R}^3} e^{-i\sqrt{\lambda - E^\alpha} \omega \cdot x} f(x) dx.$$

Then $F_{0\alpha}$ is a unitary operator from $L^2(\mathbf{R}^3)$ to $L^2((E^\alpha, \infty); L^2(S^2))$. Let

$$\hat{S}_{0\alpha} = F_0 S_{0\alpha} F_{0\alpha}^*.$$

Then for any $\lambda > 0$, there exists a bounded operator

$$\hat{S}_{0\alpha}(\lambda) \in \mathbf{B}(L^2(S^2); L^2(S^5))$$

such that

$$(\hat{S}_{0\alpha} f)(\lambda, \theta) = (\hat{S}_{0\alpha}(\lambda) f(\lambda, \cdot))(\theta)$$

for all $\lambda > 0, \theta \in S^5$ and $f \in L^2((E^\alpha, \infty); L^2(S^2))$. This is called the S-matrix. One does not know so much about its properties. The general result known so far is that of Amrein-Pearson-Sinha [A-P-S] asserting that $\hat{S}_{0\alpha}(\lambda)$ is a Hilbert-Schmidt operator for *a.e.* $\lambda > 0$. We study more detailed properties of this operator. Let

$$X_\beta = \{x \in X; x^\beta = 0\}$$

and define

$$M = S^5 \setminus \cup_\beta X_\beta, \quad N = S^5 \cap (\cup_\beta X_\beta).$$

THEOREM 1. (1) Suppose $\rho > 3$. Then $\hat{S}_{0\alpha}(\lambda)$ has a continuous kernel outside N :

$$\hat{S}_{0\alpha}(\lambda; \theta, \omega) \in C((0, \infty) \times M \times S^2).$$

(2) To study the behavior of $\hat{S}_{0\alpha}(\lambda; \theta, \omega)$ near N , we need a stronger decay assumption on the potential. Suppose $\rho > 5 + 1/2$. Let β be any pair and decompose $\theta \in S^5$ as $\theta = (\theta^\beta, \theta_\beta)$. Then as $|\theta^\beta| \rightarrow 0$,

$$\hat{S}_{0\alpha}(\lambda; \theta, \omega) \simeq |\theta^\beta|^{-1} A_{\beta, -1}(\lambda; \frac{\theta^\beta}{|\theta^\beta|}, \theta_\beta, \omega) + A_{\beta, 0}(\lambda; \frac{\theta^\beta}{|\theta^\beta|}, \theta_\beta, \omega),$$

where

$$\begin{aligned}
& A_{\beta,-1}(\lambda; \frac{\theta^\beta}{|\theta^\beta|}, \theta_\beta, \omega) \\
&= \sum_i^{finite} C_{\beta 1}^{(i)}(\lambda; \theta_\beta, \omega) \times \int_{\mathbf{R}^3} \frac{\theta^\beta}{|\theta^\beta|} \cdot x^\beta V_\beta(x^\beta) u_\beta^{(i)}(x^\beta) dx^\beta \\
&+ C_{\beta 2}(\lambda; \theta_\beta, \omega) \times \int_{\mathbf{R}^3} V_\beta(x^\beta) \psi_\beta(x^\beta) dx^\beta,
\end{aligned}$$

$u_\beta^{(i)}$ being the eigenfunction with 0 eigenvalue for h^β , and ψ_β the 0-resonance. $A_{\beta,-1} = 0$, if 0 is neither an eigenvalue nor the resonance for h^β . In this case, $\hat{S}_{0\alpha}(\lambda; \theta, \omega)$ is continuous at $\theta^\beta = 0$.

We are interested in the coefficients $C_{\beta 1}^{(i)}(\lambda; \theta_\beta, \omega)$ and $C_{\beta 2}(\lambda; \theta_\beta, \omega)$.

THEOREM 2. $C_{\beta 1}^{(i)}(\lambda; \theta_\beta, \omega)$ and $C_{\beta 2}(\lambda; \theta_\beta, \omega)$ are the scattering amplitudes for two cluster scattering.

More precisely, $C_{\beta 1}^{(i)}(\lambda; \theta_\beta, \omega)$ and $C_{\beta 2}(\lambda; \theta_\beta, \omega)$ are the scattering amplitudes for 2-cluster scattering in which, after the collision, the pair β becomes the bound state with zero energy or the zero-resonance, respectively.

Our next aim is to relate the above S-matrix to the asymptotic behavior at infinity of the generalized eigenfunction for H given by

$$\begin{aligned}
(1.1) \quad \varphi(x, \lambda, \omega) &= e^{i\sqrt{\lambda-E^\alpha}\omega \cdot x_\alpha} \varphi^\alpha(x^\alpha) + v, \\
v &= -R(\lambda + i0)f, \quad R(z) = (H - z)^{-1}, \\
f &= \sum_{\gamma \neq \alpha} V_\gamma(x^\gamma) \varphi^\alpha(x^\alpha) e^{i\sqrt{\lambda-E^\alpha}\omega \cdot x_\alpha}.
\end{aligned}$$

The first term of the right-hand-side of (1.1) corresponds to the incident wave and the next term to the scattered wave. As in the 2-body case, the S-matrix is obtained from the asymptotic behavior of v .

THEOREM 3. Suppose that $\rho > 3$. Then we have

$$s - \lim_{r \rightarrow \infty} r^{5/2} e^{-i\sqrt{\lambda}r} v(r) = C_1(\lambda) \hat{S}_{0\alpha}(\lambda; \cdot, \omega) \quad \text{in } L_{loc}^2(M).$$

It is not easy to replace M by S^5 in the above theorem, since in a neighborhood of N the behavior of v is rather complicated. We introduce a pseudo-differential operator P with symbol $p(x, \xi_\beta)$ such that

$$p(x, \xi_\beta) = \chi_\beta(x) \psi(|\xi_\beta|^2) \rho_+\left(\frac{x_\beta}{|x_\beta|} \cdot \frac{\xi_\beta}{|\xi_\beta|}\right),$$

where $\chi_\beta(x) = 1$ if $|x^\beta|/|x| < \epsilon_1$, $\chi_\beta(x) = 0$ if $|x^\beta|/|x| > 2\epsilon_1$, $\psi(t) = 1$ if $|t - \lambda| < \epsilon_2$, $\psi(t) = 0$ if $|t - \lambda| > 2\epsilon_2$, $\rho_+(t) = 1$ if $t > 1 - \epsilon_3$, $\rho_+(t) = 0$ if $t < 1 - 2\epsilon_3$, $\epsilon_1, \epsilon_2, \epsilon_3$, being small positive constants such that ϵ_1/ϵ_2 is sufficiently small. We also take $\rho(t) \in C^\infty(\mathbf{R}^1)$ such that $\rho(t) = 1$ if $1 < t < 2$, $\rho(t) = 0$ if $t < 1$ or $t > 3$. The following theorem is an analogy of Theorem 3 in a generalized sense.

THEOREM 4. *Suppose that $\rho > 5 + 1/2$. Then we have*

$$\begin{aligned} & s - \lim_{R \rightarrow \infty} \frac{1}{R} \int_{\mathbf{R}^6} e^{-i\sqrt{\lambda}\theta \cdot x} \cdot \hat{x} \rho\left(\frac{|x|}{R}\right) (Pv)(x) dx \\ & = C_2(\lambda) \hat{S}_{0\alpha}(\lambda; \theta, \omega), \quad \hat{x} = x/|x| \end{aligned}$$

in $L^2(N_\beta)$, where N_β is a small neighborhood of $N \cap X_\beta$ in S^5 .

2. Resolvent estimates

The basic estimate needed to prove the above theorems is that of Skibsted [S] established recently. Let P be a pseudo-differential operator with symbol $p(x, \xi)$ having the following properties:

$$(2.1) \quad \begin{aligned} & |\partial_x^m \partial_\xi^n p(x, \xi)| \leq C_{mn} \langle x \rangle^{-m}, \\ & \text{there exists a cone } \Gamma \subset X - \cup_\beta X_\beta \text{ such that} \\ & \text{supp}_x p(x, \xi) \subset \Gamma, \\ & \text{there exists a constant } 0 < \epsilon < 1 \text{ such that} \\ & p(x, \xi) = 0 \text{ if } \hat{x} \cdot \hat{\xi} > 1 - \epsilon. \end{aligned}$$

Then we have ([S])

$$(2.2) \quad \langle x \rangle^s PR(\lambda + i0) \langle x \rangle^{-s-t} \in \mathbf{B}(L^2(X); L^2(X))$$

if $s > -1/2, t > 1$.

To prove Theorem 1, We use the method of [I-K]. Namely, we localize the S-matrix in the phase space and apply (2.2). The singularities of $\hat{S}_{0\alpha}(\lambda; \theta, \omega)$ arise from the low-energy asymptotics of the resolvents of

2-body subsystems studied by Jensen-Kato [J-K].

To prove Theorems 3 and 4, we use the idea of the spectral representation of 2-body Schrödinger operators developed by Jäger, Ikebe, Saito and Isozaki. But we further need the following estimate.

Let $\chi_\alpha(x) = 1$ if $|x^\alpha|/|x| < \epsilon$, $\chi_\alpha(x) = 0$ if $|x^\alpha|/|x| > 2\epsilon$. Let $P_\alpha(x_\alpha, D_{x_\alpha})$ be the pseudo-differential operator with symbol $p(x_\alpha, \xi_\alpha)$ such that

$$(2.3) \quad \begin{aligned} |\partial_{x_\alpha}^m \partial_{\xi_\alpha}^n p(x_\alpha, \xi_\alpha)| &\leq C_{mn} \langle x_\alpha \rangle^{-m}, \\ p(x_\alpha, \xi_\alpha) &= 0, \text{ if } \frac{x_\alpha}{|x_\alpha|} \cdot \frac{\xi_\alpha}{|\xi_\alpha|} > \mu_- \quad (-1 < \mu_- < 1), \\ p(x_\alpha, \xi_\alpha) &= 0, \text{ if } ||\xi_\alpha| - \sqrt{\lambda}| > \epsilon_1, \quad (\epsilon_1 \ll 1). \end{aligned}$$

Then we have

$$(2.4) \quad \begin{aligned} \langle x \rangle^s \chi_\alpha(x) P_\alpha(x_\alpha, D_{x_\alpha}) R(\lambda + i0) \langle x \rangle^{-s-t} \\ \in \mathbf{B}(L^2(X); L^2(X)) \end{aligned}$$

if $s > -1/2, t > 1$.

3. Micro-local positivities and resolvent estimates

We explain the idea of the proof of (2.4). To make the arguments clear we first explain it in the case of the 2-body Schrödinger operators. We introduce the following class of symbols.

DEF. 3.1 $p(x, \xi) \in S_-^m \iff$

$$|\partial_x^\alpha \partial_\xi^\beta p(x, \xi)| \leq C_{\alpha\beta} \langle x \rangle^{m-|\alpha|} \text{ and}$$

$$p(x, \xi) = 0 \text{ if } \hat{x} \cdot \hat{\xi} > 1 - \epsilon \quad (0 < \epsilon < 1).$$

DEF. 3.2. $p(x, \xi) \in S^{-N} \iff$

$$|\partial_x^\alpha \partial_\xi^\beta p(x, \xi)| \leq C_{\alpha\beta} \langle x \rangle^{-N-|\alpha|}.$$

$p(x, \xi) \in S_-^{2m}$ is said to be a symbol of canonical type if

$$p(x, \xi) = (|x||\xi| - x \cdot \xi)^{2m} \rho(\hat{x} \cdot \hat{\xi}) \varphi(\xi) \chi(x)$$

where $\rho(t) \geq 0$, $\rho(t) = 1$ if $t < 1 - 2\epsilon$, $\rho(t) = 0$ if $t > 1 - \epsilon$, $\rho'(t) \leq 0$, $\varphi \in C_0^\infty(\mathbf{R}^n - \{0\})$, $\varphi \geq 0$, $\chi(x) \geq 0$, $\chi(x) = 1$ if $|x| > 2$, $\chi(x) = 0$ if $|x| < 1$. A simple computation shows the following lemma.

LEMMA 3.3. Let $m > -1/2$ and $p(x, \xi) \in S_-^{2m}$ be a symbol of canonical type. Let $a(x, \xi) = (|x||\xi| - x \cdot \xi)p(x, \xi)$. Then there exists a constant $C_0 > 0$ such that

$$-\{|\xi|^2, a\} \geq C_0 p + q,$$

where $\{ , \}$ denotes the poisson bracket and q is compactly supported in x .

Let $H = -\Delta + V$ be the Schrödinger operator on \mathbf{R}^n where V is a real function satisfying

$$\partial_x^\alpha V = O(\langle x \rangle^{-|\alpha|-\rho}), \quad 0 < \rho < 1.$$

Let p and a be as in Lemma 3.3 and set $A = a^W(x, D_x)$, $P = p^W(x, D_x)$. Then by Lemma 3.3, we easily have

LEMMA 3.4. $C_0 P \leq -i[H, A] + P_1 + P_N$, where $P_1 \in S_-^{2m-\rho}$, $P_N \in S^{-N}$, N being a sufficiently large constant.

Let $u = (H - z)^{-1}f$, $\text{Im}z > 0$. Then by Lemma 3.4 we have

$$(3.1) \quad C_0(Pu, u) \leq -i([H, A]u, u) + (P_1u, u) + (P_Nu, u).$$

The first term of the right-hand side is calculated as

$$(3.2) \quad -i([H, A]u, u) = -2\text{Im}z(Au, u) - i\{(Au, f) - (f, Au)\}.$$

By Garding's inequality the first term of the right-hand side of (3.2) is dominated by

$$(3.3) \quad (P_1u, u) + (P_Nu, u), \quad P_1 \in S_-^{2m-1}, \quad P_N \in S^{-N}.$$

We also have

$$(3.4) \quad |(Au, f)| \leq \frac{1}{2}(\|Au\|_{-m-1-\rho}^2 + \|f\|_{m+1+\rho}^2) \\ \leq (P_1u, u) + C\|f\|_{m+1+\rho}^2, \quad P_1 \in S_-^{2m-2\rho}.$$

These estimates together with (3.1) show that

$$(3.5) \quad (Pu, u) \leq (P_1u, u) + C\|f\|_{m+1+\rho}^2, \quad P_1 \in S_-^{2m-\rho}.$$

Here we note that the symbol of $P_1 \in S_-^{2m-\rho}$ is dominated from above by the symbol of canonical type $\in S_-^{2m-\rho}$. So, one can use (3.5) with $2m$ replaced by $2m - \rho$ to estimate $(P_1 u, u)$. We repeat this procedure and finally obtain

$$(Pu, u) \leq C \|f\|_{m+1+\rho}^2,$$

which implies that

$$\|Pu\|_m \leq C \|f\|_{m+1+\rho},$$

if $P \in S_-^m$, $m > -1/2$.

Now we turn to the three body problem and give the idea to prove the estimate (2.4). We introduce S_-^m , P , A in the same way as in the 2-body case with x , ξ replaced by x_α , ξ_α . Let $u = R(z)f$, $z = \lambda + i\epsilon$. Since

$$-i[H, \chi_\alpha A \chi_\alpha] = -i\chi_\alpha [H, A] \chi_\alpha - i[H, \chi_\alpha] A \chi_\alpha - i\chi_\alpha A [H, \chi_\alpha],$$

we have

$$C_0(\chi_\alpha P \chi_\alpha u, u) \leq -i(\chi_\alpha [H, A] \chi_\alpha u, u) + (\chi_\alpha P_1 \chi_\alpha u, u) + \dots$$

with $P_1 \in S_-^{2m-\rho}$. Let $\varphi(\cdot)$ be a smooth cut off function near λ . Then

$$[H, \chi_\alpha] A \chi_\alpha R(z)f = [H, \chi_\alpha] A \chi_\alpha \varphi(H_0) R(z)f + \text{lower order term}.$$

Now we note that on the support of the symbol of $[H, \chi_\alpha] A \chi_\alpha \varphi(H_0)$, $x \cdot \xi \leq \mu_- |x| |\xi|$, $-1 < \mu_- < 1$, which follows from the fact that $x_\alpha \cdot \xi_\alpha < (1 - \epsilon) |x_\alpha| |\xi_\alpha|$. So, one can apply the estimate (2.2) to control this term. The rest of the proof is the same as in the 2-body case.

4. References

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